Liang Wang

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Education

National University of Singapore — **Singapore**
Visiting Ph.D. Student — *2025 - 2026 (expected)*

- Lab: ZhangLab
- Advisor: Prof. Yang Zhang Mentor: Dr. Zhiyuan Liu
- Research Interests: AI for Science, Diffusion Models, LLM Reasoning

Institution of Automation, Chinese Academy of Sciences — **Beijing, China**
Ph.D. in Pattern Recognition and Intelligent Systems (selected for the PhD honors program) — *2021 - 2026 (expected)*

- Lab: State Key Laboratory of Multimodal Artificial Intelligence Systems (MAIS)
- Advisor: Prof. Liang Wang Co-advisors: Prof. Shu Wu and Prof. Qiang Liu
- Research Interests: AI for Science, Graph Machine Learning, Data Mining

Tongji University — **Shanghai, China**
B.Eng. in Software Engineering — *2017 - 2021*

- GPA: 4.86/5.00 (Ranking 3/214, Top 1.4%)
- Honors and Awards: National Scholarship (Top 1%), Outstanding Graduate of Shanghai (Top 5%)

Selected Publications

MolSpectra: Pre-training 3D Molecular Representation with Multi-modal Energy Spectra
- Liang Wang, Shaozhen Liu, Yu Rong, Deli Zhao, Qiang Liu, Shu Wu, Liang Wang
- *ICLR 2025*

Pin-Tuning: Parameter-Efficient In-Context Tuning for Few-Shot Molecular Property Prediction
- Liang Wang, Qiang Liu, Shaozhen Liu, Xin Sun, Shu Wu, Liang Wang
- *NeurIPS 2024*

Rethinking Graph Masked Autoencoders through Alignment and Uniformity
- Liang Wang*, Xiang Tao*, Qiang Liu, Shu Wu, Liang Wang
- *AAAI 2024*

Bi-Level Graph Structure Learning for Next POI Recommendation
- Liang Wang, Shu Wu, Qiang Liu, Yanqiao Zhu, Xiang Tao, Mengdi Zhang, Liang Wang
- *IEEE Transactions on Knowledge and Data Engineering 2024*

DIVE: Subgraph Disagreement for Graph Out-of-Distribution Generalization
- Xin Sun, Liang Wang, Qiang Liu, Shu Wu, Zilei Wang, Liang Wang
- *KDD 2024*

GSLB: The Graph Structure Learning Benchmark
- Zhixun Li, Liang Wang, Xin Sun, Yifan Luo, Yanqiao Zhu, Dingshuo Chen, Yingtao Luo, Xiangxin Zhou, Qiang Liu, Shu Wu, Liang Wang, Jeffrey Xu Yu
- *NeurIPS 2023*

Semantic Evolvement Enhanced Graph Autoencoder for Rumor Detection
- Xiang Tao, Liang Wang, Qiang Liu, Shu Wu, Liang Wang
- *WWW 2024*

S^{2}DN: Learning to Denoise Unconvincing Knowledge for Inductive Knowledge Graph Completion
- Tengfei Ma, Yujie Chen, Liang Wang, Xuan Lin, Bosheng Song, Xiangxiang Zeng
- *AAAI 2025 (Oral)*

Chain-of-History Reasoning for Temporal Knowledge Graph Forecasting
- Yuwei Xia, Ding Wang, Qiang Liu, Liang Wang, Shu Wu, Xiaoyu Zhang
- *ACL 2024 (Findings)*

Preprint Papers

1. **Diffusion Models for Molecules: A Survey of Methods and Tasks**
   - Liang Wang, Chao Song, Zhiyuan Liu, Yu Rong, Qiang Liu, Shu Wu, Liang Wang
   - *arXiv preprint 2025*

2. **Materials Generation in the Era of Artificial Intelligence: A Comprehensive Survey**
   - Zhixun Li*, Bin Cao*, Rui Jiao*, Liang Wang*, Ding Wang, Yang Liu, Dingshuo Chen, Jia Li, Qiang Liu, Yu Rong, Liang Wang, Tong-yi Zhang, Jeffrey Xu Yu
   - *arXiv preprint 2025*

3. **A Survey of Graph Transformers: Architectures, Theories and Applications**
   - Chaohao Yuan, Kangfei Zhao, Ercan Engin Kuruoglu, Liang Wang, Tingyang Xu, Wenbing Huang, Deli Zhao, Hong Cheng, Yu Rong
   - *arXiv preprint 2025*

Selected Projects

PyGCL: A PyTorch Library for Graph Contrastive Learning **https://github.com/PyGCL/PyGCL**

- ☆ Github Star: 943
- An easy-to-use library for graph contrastive learning with PyTorch. It implements a wide variety of contrastive objectives, data augmentations, contrasting modes and other utilities useful for implementing and evaluating contrastive learning on graphs.

GSLB: A Benchmark of Graph Structure Learning **https://github.com/GSL-Benchmark/GSLB**

- ☆ Github Star: 116
- An open-source library built for easy implementation and evaluation of graph structure learning model family. It offers a versatile control of graph dataset laoding, structure learners, structure processors, and a bunch of reproduced models.

Internship

DP Technology **Beijing, China**

Research Intern (Remote) *Apr. 2025 - Now*

- Conducting research on large language models for reasoning and planning complex scientific problems using reinforcement learning.

AI4Science Group, Alibaba DAMO Academy **Hangzhou, China**

Research Intern *Aug. 2024 - Mar. 2025*

- Advised by Dr. Yu Rong and Dr. Tingyang Xu.
- Conducted research on AI for chemistry and life science. The research work has been published in ICLR 2025.

Graph Learning Group, NLP Center, Meituan Inc. **Beijing, China**

Research Intern *Sept. 2021 - Oct. 2022*

- Conducted research on graph self-supervised learning and graph-based spatial-temporal data mining. The research works have been published in IEEE TKDE and SDM 2024.

Advertising Department, ByteDance Inc. **Shanghai, China**

Machine Learning Engineer Intern *Jul. 2020 - Dec. 2020*

- Supported the improvement of advertising machine learning models, and the development of the advertising system.

Talks

Molecular Spectroscopy, at Alibaba DAMO Academy, 2024, Slides
Molecular Representation Learning and Property Prediction, Invited by DP Technology, 2024, Slides
Denoising-based 3D Molecular Pre-training, 2024, Slides
Generative Graph Self-Supervised Learning, 2023, Slides
Graph Transformers, 2022, Slides
Graph Self-Supervised Learning and Pre-Training, 2021, Slides

Academic Services

Conference Reviewers

- Conference on Neural Information Processing Systems (NeurIPS), 2024, 2025
- International Conference on Learning Representations (ICLR), 2025
- International Conference on Machine Learning (ICML), 2025
- ACM SIGKDD Conference on Knowledge Discovery and Data Mining (KDD), 2024, 2025
- International Conference on Artificial Intelligence and Statistics (AISTATS), 2025

Journal Reviewers

- IEEE Transactions on Knowledge and Data Engineering (TKDE)
- IEEE Transactions on Computational Biology and Bioinformatics (TCBB)

Technical Skills

Programming Languages: Python, C++, Java, Go, C#, Matlab
Machine Learning Frameworks: PyTorch, PyTorch Geometric (PyG), Deep Graph Library (DGL), Hugging Face Transformers, Hugging Face Diffusers
Others: LaTeX, Git